University of Virginia, Department of Materials Science and Engineering

Spring 2006, Tuesday and Thursday, 9:30-10:45 am
Materials Science Building, Room 125

MSE 524: Modeling in Materials Science

Instructor: Leonid V. Zhigilei
Office: Materials Science Building 227
Office hours: open
Telephone: (434) 243-3582
E-mail: lz2n@virginia.edu

Web page: http://www.faculty.virginia.edu/CompMat/

Abstract: The course provides an overview of Computational Materials Science, a relatively new and one of the fastest growing disciplines in Materials Science. Computational (primarily classical) methods of atomistic, mesoscopic, continuum, and multiscale modeling will be discussed in the context of real materials-related problems (mechanical and thermodynamic properties, phase transformations, microstructure evolution during processing). Success stories and limitations of contemporary computational methods will be considered.

The emphasis of the course will be on getting practical experience in designing and performing computer simulations. Pre-written codes implementing atomistic computational methods will be provided. Students will use and modify the pre-written codes and write their own simulation and data analysis codes while working on their homework assignments and term projects. A set of example problems for term project will be provided although students are encouraged to choose a project relevant to their thesis research.

Recent research articles in the area of Computational Materials Science will be discussed. Students will learn to assess the quality and significance of published computational works.

Grading: Term project 50%
Homeworks 40%
Presentation/discussion of published research articles 10%

Homework:
Homework does not require the pledge and cooperation among students (preferably through course e-mail list) is permitted.

Main text: Handouts and lecture notes.

Books placed on reserve circulate in the Engineering Library:

1. D. Raabe, Computational materials science: the simulation of materials microstructures and properties (Wiley-VCH: Weinheim, New York, 1998). Call number: TA403.6 .R23 1998

2. M. P. Allen and D.J. Tildesley, Computer simulation of liquids (Clarendon Press: Oxford, 1990, 1987). Call number: QC 145.2 .A43 1990 or QC145.2 .A43 1987

3. D. Frenkel and B. Smit, Understanding molecular simulation: from algorithms to applications (Academic Press: San Diego, 1996). Call number: QD461 .F86 1996

4. M. Metcalf and J. Reid, Fortran 90/95 explained (Oxford University Press: Oxford, New York, 1999). Call number: QA76.73 .F28 M49 1999

Additional books:

Jörg-Rüdiger Hill, Lalitha Subramanian, and Amitesh Maiti, Molecular modeling techniques in material sciences (Taylor & Francis/CRC Press: Boca Raton, FL, 2005). Call number: TA401.3 .H55 2005

Handbook of Materials Modeling, edited by Sidney Yip (Springer, Berlin, New York, 2005).

M. Meyer and V. Pontikis, Computer simulation in materials science: interatomic potentials, simulation techniques, and applications (Kluwer Academic: Boston, 1991). Call number: TA 403.6 .N42 1991

V. Bulatov, T. Diaz de la Rubia, R. Phillips, T. Kaxiras, and N.M.Ghoniem, Multiscale Modelling of Materials (Mat. Res. Soc. Symp. Proc. v. 538, MRS: Warrendale, Pa., 1999). Call number: TA405 .M887 1999

W. G. Hoover, Computational statistical mechanics (Elsevier: Amsterdam, New York, 1991). Call number: QC 174.8 .H66 1991

K. Ohno, K. Esfarjani, and Y. Kawazoe, Introduction to computational materials science: from ab initio to Monte Carlo methods (Springer-Verlag: Berlin, New York, 1999). Call number: TA404.23 .O36 1999

H. Kitagawa, T. Aihara Jr., Y. Kawazoe, Mesoscopic dynamics of fracture: computational materials design (Springer-Verlag: Berlin, New York, 1998). Call number: TA409 .M458 1998

K. Binder and D.W. Heermann, Monte Carlo simulation in statistical physics: an introduction (Springer: Berlin, New York, 1997). Call number: QC174.85 .M64 B56 1997

K. Binder, Monte Carlo and molecular dynamics simulations in polymer sciences (Oxford University Press: Oxford, New York, 1995). Call number: QD 381.9 .E4 M66 1995

T. Saito, Computational materials design (Springer: Berlin, New York, 1999). Call number: TA404.8 .C66 1999

W. H. Press, et al., Numerical Recipes in Fortran 90 (or C): The Art of Scientific and Parallel Computing, Cambridge University Press, is available on-line from http://www.nr.com/

Topics that are covered include:

- Introduction
  - Spatial and temporal hierarchy of microstructure and dynamics in materials
  - Types of models: quantum mechanical, atomistic, mesoscopic, continuum
  - Multiscale approaches

- Short review and elements of differential equations (numerical solution)
  - Differential equations in discrete and continuum simulation methods
  - Ordinary differential equations for particle dynamics
  - Partial differential equations, conduction/diffusion equation

- Atomistic models: Molecular dynamics
  - The basics of classical molecular dynamics
  - Initial conditions, creating lattice structures, introducing defects
  - Defining and maintaining temperature and pressure
  - Boundary conditions (periodic, stochastic, conducting, non-reflecting)
  - Methods for constant temperature or/and pressure simulations
  - Tricks of the trade (neighbor lists, force/energy tables, potential cutoffs, etc.)

- Monte Carlo methods
  - The basics of Monte Carlo
  - Monte Carlo integration, thermodynamic averages
  - Importance sampling, Metropolis scheme
  - Lattice Monte Carlo, Ising model
  - Multi-state Potts models (grain coarsening, recrystallization)
  - Kinetic Monte Carlo (surface processes, thin film growth)

- Interatomic potentials
  - Introduction, Born-Oppenheimer approximation
  - Pair potentials and their limitations
  - Calculation of elastic constants from potential function
  - Potentials for ionic systems, ceramics
  - Many-body potentials for metals
  - Many-body potentials for covalently bounded systems
  - *Forces from "first principles" (time permitting)*

- Analysis of the simulation results
  - Equilibrium properties (energy, temperature, pressure, velocity distributions)
  - Structural properties (geometrical tessellation, pair correlation functions, atomic-level stresses)
  - Dynamic properties (diffusion, time correlation functions)

- Mesoscopic methods
  - Discrete dislocation dynamics
    - Strain and stress fields for edge and screw dislocations in an isotropic medium
    - The equation of motion in Newtonian Dislocation Dynamics
    - Examples from 2D and 3D simulations
    - Current problems
  - *Coarse-grained models for organic materials (time permitting)*

- Bridging the scale gaps between different simulation levels
  - Simultaneous integration of the models
  - Sequential integration of the models (hierarchical approach)
  - Examples of combined methods (MD-FEM, MD-MC, etc.)

- Computer use
  - Introduction to UNIX and Networking (if needed)
  - Visualization (VRML, Java-applets, animated gifs, animations with Tecplot)

- Codes to be provided
  - MSE524-MD code for MD simulations
  - MSE524-CG crystal generator (FCC, BCC, diamond)
  - MSE524-MC Ising model for binary alloys
  - An example VRML code for visualization of an atomic structure

Discussion of published research articles

Each student will lead one or two discussions of recent research papers in the area of Computational Materials Science (~10-15 min). Although a few papers will be proposed by instructor, students are encouraged to propose papers that are interesting or relevant to their research work (but not to the term project). Papers should be posted on the course web site at least one week before the discussion.

Term project

Objective: To get experience in designing and performing computer simulations.

Parts of the project:
- Design (or adapt an idea from literature) a simulation that is of scientific or computational interest to you
- Justify what computational approach is appropriate
- Write a computer code (or add parts to MSE524-MD code)
- Perform simulations and analyze the results
- Prepare a report; include electronic copies of your code
- Make a short presentation to the class (mini-symposium)

Timeline:
February 9th - have project approved by instructor
March 2nd – turn in introduction and discuss progress with instructor
May 4th – turn in a report; give a presentation to the class at a mini-symposium

Sample projects:
A set of example problems for term project will be given. A problem chosen for the term project should have some science content and be doable in the timeframe of one semester. Students are encouraged to choose a project relevant to their thesis research. If the intention is to continue computational work in the future, the term project may be a well-defined part of a larger research project.